HPV Challenge Program
Final Report
For

1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H) -trione

CAS No. 27676-62-6

The American Chemistry Council
Rubber and Plastic Additives Panel

May 22, 2006

Executive Summary

A. Introduction

An important objective of EPA's High Production Volume (HPV) chemical challenge program is the gathering and public release of basic hazard information on those chemicals manufactured at high volumes in the United States. The American Chemistry Council, Rubber and Plastic Additives Panel, is participating in this program and hereby submits our available data for 1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione. Within the panel, this compound is sponsored by Ciba Specialty Chemicals Corporation and Noveon, Inc.

B. General Substance Information

Chemical Name: 1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione

Appearance: White to off-white powder.

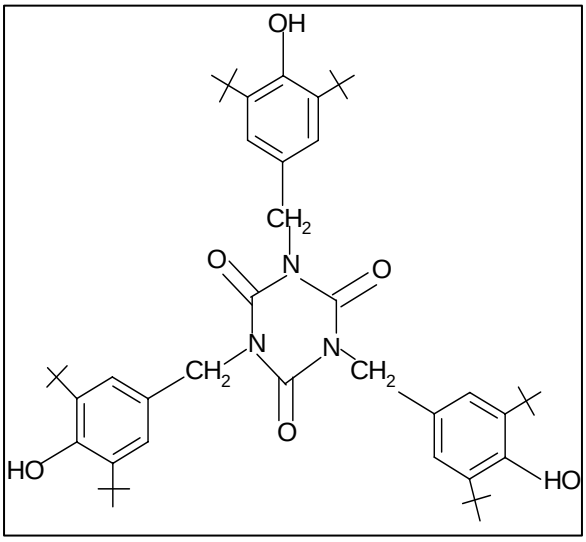
Chemical abstract Service Registry Number: CAS # 27676-62-6

Common Name / Trade Name: Irganox 3114

Chemical Formula: C48H69N3O6

Molecular weight: 784

Structure:



C. General Use Information

1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6 (1H,3H,5H)-trione is a sterically hindered phenolic antioxidant. The compound is a stabilizer for organic substrates such as polymers, synthetic fibers, elastomers, adhesives, waxes, oils and fats. It protects these substrates against thermo-oxidative degradation and contributes to their light stability.

This product has been cleared by the FDA for use in various polymers and adhesives intended for food contact applications [21 CFR § 178.2010 and 175.105].

Sales of the product are to industrial users only. The polymer industry has a record of safe use of such additives and worker exposures are considered minimal. Industrial hygiene programs and Responsible Care® practices are the norm throughout the industry and it is our experience that users handle such products in a careful and conscientious manner. Material Safety Data Sheets (MSDS) are distributed that present detailed hazard data and provide directions for safe handling.

The product can be used in polyolefins, namely polyethylene, polypropylene, polybutene as well as other polymers such as styrene homo- and copolymers. It may also be used in linear polyesters, PVC, polyamides and polyurethanes, elastomers such as SBS, EPR, EPDM, and other synthetic rubbers, adhesives, natural and synthetic tackifier resins and other organic substrates. In polyolefins, the concentration levels range typically between 0.05% and 0.3% depending on substrate, processing conditions and long-term thermal stability requirements. The optimum level is application specific.

This compound has good compatibility with most substrates, high resistance to extraction and low volatility. It is odorless and stable to light. The product can be used in combination with other additives such as costabilizers, light stabilizers and other functional stabilizers. After incorporation in the polymer matrix it is relatively immobile and release-exposure to humans or the environment is considered minimal.

Environmental Endpoints

Existing ecotoxicology data for this chemical indicate that there is low concern for acute toxicity to fish, aquatic plants and aquatic invertebrates. The material is not readily biodegradable, however, environmental exposures are expected to be negligible and a low potential for bioaccumulation is indicated. Aquatic Toxicology experimental data are available on acute fish toxicity, acute invertebrate toxicity, and alga toxicity for this chemical.

Toxicology Endpoints

Available mammalian acute toxicity data indicates very low toxicity by oral and dermal exposure. The LD50 values are >5000 mg/kg bw (oral) and >2000 mg/kg bw (dermal). The material does not show mutagenic or clastogenic properties. In sub-chronic toxicity studies in the rat and dog only minor effects have been observed. The substance was

found to be neither carcinogenic nor a reproductive toxicant. A rat developmental toxicity study (OECD 414) conducted for the HPV program showed that the compound is not teratogenic (NOEL Maternal Toxicity: 1000mg/kg/day, NOEL Teratogenicity: 1000 mg/kg/day).

Conclusions

With the recent completion of a rat developmental toxicity study, there are no data gaps for 1,3,5–tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione. The available data are sufficient to meet the requirements of the HPV challenge program. The existing chemistry, ecotoxicity and mammalian toxicity testing demonstrates that the compound poses acceptably low risks to man and the environment for its present commercial use as an antioxidant stabilizer.

SUMMARY TABLE

CAS No. 27676-62-6 **PHYSICAL/CHEMICAL ELEMENTS**	**DATE**	**RESULTS**	**FULFILLS REQUIREMENT**
Melting Point	2002	219.5-225.5 ^{o}C	Yes
Boiling Point	2001	960.98 ^{o}C	Yes
Vapor Pressure	2002	5 x 10^{-15} mm Hg	Yes
Partition Coefficient	2002	log P > 6.0	Yes
Water Solubility	2002	< 1 ppm	Yes
ENVIRONMENTAL FATE ELEMENTS			
Photodegradation	2001	For reaction with hydroxyl radical, predicted rate constant = 66.5 x 10^{12} cm^3/molecule-sec predicted half-life = 1.93 h	Yes
Stability in Water	2001	Hydrolysis rate extremely slow	Yes
Fugacity	2001	Predicted distribution using Level III fugacity model Air 0.02 % Water 1.15 % Soil 38.4 % Sediment 60.4 % Persistence = 6.4 x 10^3 h	Yes
Biodegradation	1985	Not biodegradable 0 -7 % after 28 days	Yes
Bioaccumulation	2001	Estimated log BCF = 0.50 (BCF = 3.16)	
ECOTOXICITY ELEMENTS			
Acute Toxicity to Fish	1988	Zebra fish (Brachydanio rerio): LC_{50} (24 – 96 h) => 100 mg/L	Yes
Toxicity to Aquatic Plants	1992	Green algae (Scenedesmus subspicatus): EC_{50} (0 – 72 h) => 100 mg/L NOEC (0 – 72 h) = 33 mg/L	Yes
Acute Toxicity to Aquatic Invertebrates	1988	Daphnia magna: EC_0 (24 h) = > 100 mg/L EC_{50} (24 h) = 32 mg/L EC_{100} (24 h) => 100 mg/L	Yes

SUMMARY TABLE (CONTINUED)

CAS No. 27676-62-6 HEALTH ELEMENTS	DATE	RESULTS	FULFILLS REQUIREMENT
Acute Toxicity	1986	Rat: LD_{50} (Oral) > 5000 mg/kg	Yes
	1992	Rabbit: LD_{50} (Dermal) > 2000 mg/kg	Yes
Genetic Toxicity in vivo	1987	Chinese hamster: Nonmutagenic in somatic mutation assay (exposed by gavage 5000 mg/kg)	Yes
Genetic Toxicity in vitro	1986	Salmonella typhimurium: No increase in mutations with or without metabolic activation (at doses of 20 – 5000 µg/0.1 mL)	Yes
	1978	Salmonella typhimurium: No increase in mutations with or without metabolic activation (at doses of 25 – 2025 µg/0.1 mL)	Yes
Genetic Toxicity in vitro (non-bacterial)	1991	Chinese hamster V79 cells: No increase in mutations with or without metabolic activation (at doses of 27.5 – 550 µg/0.1 mL)	Yes
Cytogenetic test	1991	Chinese hamster ovary cells: No clastogenic effects	Yes
Repeated Dose Toxicity	1990	Albino Rats: NOEL = 3000 ppm (males) NOEL = 800 ppm (females) (90 days exposure, diet)	Yes
	1970	Albino Rats: NOEL = 10,000 ppm (92-93 days exposure, diet)	
	1970	Dog: NOEL = 10,000 ppm (90 days exposure, diet)	
Developmental Toxicity	2005	NOEL Maternal Toxicity: 1000mg/kg/day NOEL Teratogenicity: 1000 mg/kg/day	Yes
Toxicity to Reproduction	1970-90	90-day repeat dose studies provide appropriate data on reproductive organs	Yes
Chronic Toxicity / Carcinogenicity	1978	2 year rat study: Not carcinogenic at 100 ppm	Yes